Indian J. Phys. **48**, 1141–1143 (1974).

Crystallographic data of hydrazobenzene

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(*Received* 8 *December* 1973, *revised* 20 *July* 1974)

A small difference was observed (Becker & Jancke 1921) between the orientations of benzene rings in the crystal of hydrazobenzene ($C_6H_5NHNHC_6H_5$) from the optical and magnetic data. It is probably due to the fact that the mutual influences between the optical dipole moments of neighbouring molecules are quite large and not negligible. There is discrepancy in the value of the observed unit cell dimensions of hydrazobenzene crystal between Becker & Jancke (1921) and Charghade (1967). On account of this pecularity it was considered desirable to carry on a full X-ray investigation into the structure of this compound.

On account of discrepancies, as stated above, it was found necessary to carry out the experiments as accurately as possible.

The finely powdered sample was placed in a capillary tube of low absorbing glass, having wall thickness 0.01 mm and diameter 0.5 mm. Precautions were taken to avoid moisture. The powder photograph (Debye Scherrer pattern) was taken, using a camera of 11.5 cm diameter. The filtered CuK_α radiation from an X-ray tube was operated at 15 mA and 30 Kv.

Attempts were made to index the powder diffraction lines with various systems (Azaroff & Buerger 1958) and the best fittings were observed with body centred orthorhombic system having cell dimensions as follows

$$a = 7.335 \pm 0.0020\text{Å},\ b = 7.529 \pm 0.0030\text{Å} \text{ and } c = 18.714 \pm 0.0170\text{Å}.$$

There is good agreement between the observed and calculated values of $Q_{hkl} = 1/\alpha^2$ as shown in table 1.

There are three refractive indices α, β and γ. The highest refractive index, γ should be along c-axis, while α and β should be along b and a axes respectively. The optical measurements were made on the crytstal of hydrazobenzene and gave the following results

$\alpha = 1.591$ (along b axis),

$\beta = 1.605$ (along a axis), and

$\gamma = 1.710$ (along c axis).

Table 1. Index powder pattern of hydrazobenzene

Index $h\ k\ l$	Q_{hkl} (Cal)	Q_{hkl} (Obs)	Intensity
0 0 2	0.0114	—	—
0 0 4	0.0456	—	—
1 1 2	0.0477	0.0473±0.0004	W
0 2 0	0.0709	—	—
2 0 0	0.0744	0.0740±0.0004	W
0 2 2	0.0823	—	—
1 1 4	0.0819	0.0819±0.0005	W
2 0 2	0.0858	—	—
2 1 1	0.0950	0.0945±0.0005	S
0 0 6	0.1026	0.1030±0.0005	W
0 2 4	0.1165	0.1161±0.0006	W
2 1 3	0.1178	—	—
2 0 4	0.1200	—	—
1 1 6	0.1390	0.1390±0.0006	W
2 2 0	0.1453	—	—
2 2 2	0.1568	0.1562±0.0006	W
2 1 5	0.1634	0.1628±0.0007	W
0 0 8	0.1824	—	—
1 1 8	0.2187	—	—
3 1 4	0.2308	0.2291±0.0007	W
2 0 8	0.2568	—	—
3 2 3	0.2640	0.2633±0.0007	W
0 0 10	0.2850	—	—
3 1 6	0.2878	—	—
4 0 0	0.2977	—	—
3 2 5	0.3093	0.3093±0.0008	W
4 1 1	0.3183	—	—
2 1 9	0.3230	—	—
2 3 9	0.3648	—	—
3 1 8	0.3676	0.3674±0.0008	W
4 1 5	0.3807	—	—
4 0 6	0.4006	—	—
0 0 12	0.4104	0.4104±0.0008	V,W
3 1 10	0.4702	0.4704±0.0008	W
4 0 8	0.4801	—	—

Rotation and Weissenberg photographs further confirmed the above results. Hydrazobenzene crystallizes in the bipyramidal class of orthorhombic crystal.

The density of the crystal measured by floatation method, was found to be 1.179±0.001 gm/c.c. The number of molecules per unit cell was found and the calculated value of density for four molecules in the unit cell was 1.18 gm/c.c.

Space group : From this indexed oscillation and Weissenberg photographs, the following systematic absences of reflections were observed

hkl : $h+k+l = 2n$
okl : $(k+l = 2n)$
hol : $(h+l = 2n)$
hko : $(h+k = 2n)$
hoo : $(h = 2n)$
oko : $(k = 2n)$
ool : $(l = 2n)$
hko : $h = 2, \quad (k = 2n)$
hol : $l = 2n, \quad (h = 2n)$
okl : $k = 2n, \quad (l = 2n)$

and therefore, $I2_12_12_1$ was assigned as the probable space group.

Further structural details will be published in due course.

The authors express their sincerest gratitude to Dr. L. S. Sing, University Professor and Head of the University Department of Physics, Patna University, Patna-5, for his keen interest and encouragements.

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***Indian J. Phys.* 48, 1143–1145 (1974).**

On limiting density in white stars

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(*Received* 17 *December* 1973)

Using the equilibrium condition for limiting density, namely,

$$\frac{d}{dn}(E_k+E_G) = 0, \qquad \ldots (1)$$

where E_k denotes the total kinetic energy and E_G the gravitational potential energy, Stoner (1929, 1930) and Anderson (1929) determined the maximum